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Technical Report No. 35

An Examination of the Configuration Averaged Hartree-Fock Procedure for Model
Ferrodoxin and Its Electronic Spectroscopy

by

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To be Submitted for Publication

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April 19, 1995

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An Examination of the Configuration Averaged Hartree-Fock Procedure for Model Ferredoxin and Its Electronic Spectroscopy

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Abstract

A configuration averaged Hartree-Fock (CAHF) procedure has been applied to a model ferredoxin $[\text{Fe}_2\text{S}_2(\text{SH})_4]^{2-}$. The anti-ferromagnetism and spectroscopy have been studied within the restricted open-shell Hartree-Fock (ROHF) approximation and the resulting wavefunction refined by a subsequent configuration interaction (CI). The results obtained suggest that a simple CAHF model, with spin projection, is accurate, typically producing states of the correct nature when compared with those derived from far more computer intensive ROHF-CI calculations. A general procedure is proposed which allows for the calculation of the electronic spectra of either the high spin or the anti-ferromagnetic ground states using a CI for the highest multiplicity states only. The procedure we demonstrate here can be extended to more sophisticated models of ferredoxins; i.e., systems containing more metal atoms and therefore more complex multiplicity problems.

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